MODFLOW-STO: Stochastic Modeling of Flow in Saturated Porous Media Using MODFLOW-2000

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ABSTRACT

We developed a stochastic version of MODFLOW, referred to as MODFLOW-STO, for simulating flow in saturated, randomly heterogeneous porous media. The model is on the basis of an innovative combination of Karhunen-Loéve decomposition, polynomial expansion, and perturbation methods. The log conductivity (ln*K*) field is first decomposed using the Karhunen-Loéve expansion. The head *h* is then decomposed with a perturbation expansion as the sum of $h^{(m)}$, m = 0, 1, …, where $h^{(m)}$ represents the m^{th} head in σ_Y, the standard deviation of ln*K*. Term $h^{(m)}$ is further expanded into a polynomial series of *m* products of orthogonal standard Gaussian random variables whose coefficients $h^{(m)}_{i_1,i_2,\ldots,i_m}$ are deterministic and can be solved recursively from low to high orders. All equations for these coefficients share the exactly same structure with the original flow equation, which allows us to use any existing groundwater simulator, such as MODFLOW-2000, to quantify flow uncertainties. The means and variances of head and flux are calculated using simple algebraic operations on $h^{(m)}_{i_1,i_2,\ldots,i_m}$. In the current version of MODFLOW-STO, $h^{(m)}$ is solved up to the third order in σ_Y. The model has been tested under a wide range of flow conditions against the classical Monte Carlo simulations (MCS). Results indicate that MODFLOW-STO is capable of providing accurate solutions and requires much less computation effort as compared to the MCS analysis. With MODFLOW-STO, subsurface flow uncertainty can be quantified under field conditions in an efficient, effective manner.

INTRODUCTION

It has been long recognized that subsurface flow modeling is usually associated with uncertainties. In a field geologic setting, the lithologic, petrophysical and structural components often vary in such a dramatic way that cannot be predicted deterministically. Thus, the parameters (e.g., hydraulic conductivity, etc.) measured at selected locations represent each point specifically whose value depends on measuring scale as well as measuring procedures. To extend these values to those areas where measurements are not available introduces a great deal of uncertainty. Furthermore, the measurement data themselves are often corrupted by experimental and interpretive errors. These errors and uncertainties render the parameters and corresponding flow modeling to be stochastic instead of deterministic. To address subsurface flow problems under uncertainties, many stochastic approaches have emerged in the past two decades (Zhang, 2002). Current stochastic methods can be categorized as Monte Carlo simulations (MCS) or the moment equation (ME) approach. The MCS is straightforward conceptually but suffers from a heavy computational burden. Analytical solutions of the ME approach require strong simplifying assumptions and are typically not applicable for realistic problems. The computational effort in the numerical ME approach increases dramatically with the problem dimensions and is thus limited in its applicability under field conditions.

In this work we adopt a new approach proposed by Zhang and Lu (2004), called the Karhunen-Loéve decomposition-based Moment Equation (KLME), and integrate it with the USGS model MODFLOW-2000 (MF2K, Harbaugh et al., 2000). The resulting model is referred to as MODFLOW-STO. In this model, we first expand the log conductivity (ln*K*) field into a series in terms of orthogonal standard Gaussian random variables with their coefficients obtained as the eigenvalues and eigenfunctions of the covariance function of ln*K*. The head *h* is then decomposed with a perturbation expansion as the sum of $h^{(m)}$, m = 0, 1, …, where $h^{(m)}$ represents the m^{th}-order head in terms of σ_Y, the standard deviation of ln*K*. The m^{th}-order head $h^{(m)}$ is further expanded into a polynomial series of *m* products of orthogonal standard Gaussian random variables whose coefficients $h^{(m)}_{i_1,i_2,\ldots,i_m}$ are deterministic and can be solved sequentially from low to high orders. All equations for these coefficients share the exactly same structure with the original flow equation, which allows us to use MF2K as a solver directly without major modifications. The statistic moments (the means and variances) of flow quantities can then be calculated from these coefficients.

METHODOLOGY

Governing Equations

Within the MODFLOW-2000 context, the governing equation for groundwater flow under water-table conditions can be written as,

$$\nabla_{xy}\cdot[K_s(\boldsymbol{x})h_B(\boldsymbol{x},t)\nabla_{xy}h(\boldsymbol{x},t)]+K_s(\boldsymbol{x})\frac{\partial h(\boldsymbol{x},t)}{\partial z}+g_u=S_y\frac{\partial h(\boldsymbol{x},t)}{\partial t}, \qquad (1)$$

where $K_s(\boldsymbol{x})$ is the hydraulic conductivity; h is the hydraulic head; $h_B(\boldsymbol{x},t)=h(\boldsymbol{x},t)-BOT1$ is the saturated thickness; $BOT1$ is the bottom elevation of the water-table layer; g_u is the sink/source term applied to the water-table layer (e.g., recharge); S_y is specific yield; $\boldsymbol{x}$ is a vector of spatial Cartesian coordinate; t is time; and ∇_{xy} is defined as $(\partial/\partial x, \partial/\partial y)$. Note that when $BOT1$ is zero, $h_B(\boldsymbol{x},t)$ reduces to $h(\boldsymbol{x},t)$. $K_s(\boldsymbol{x})\partial h(\boldsymbol{x},t)/\partial z$ represents the Darcy's flux between the water-table and underlying confined layers in the vertical direction. For the underlying confined portions, the governing equation is written as,

$$\nabla\cdot[K_s(\boldsymbol{x})\nabla h(\boldsymbol{x},t)]+g_c=S_s\frac{\partial h(\boldsymbol{x},t)}{\partial t}, \qquad (2)$$

where g_c (1/T) is the sink/source that is applied to the confined portions; S_s is the specific storage; and ∇ stands for $(\partial/\partial x, \partial/\partial y, \partial/\partial z)$. The coupled equations (1) and (2) are solved simultaneously along with appropriate initial and boundary conditions. In the study $K_s(\boldsymbol{x})$ is taken as a random function and all other parts of the flow model are assumed to be deterministic. Our goal here is to solve for the mean heads and fluxes and the associated uncertainty expressed in terms of variances.

Karhunen-Loéve (KL) Decomposition of Hydraulic Conductivity Field

Let $Y(\boldsymbol{x})=\ln[K_s(\boldsymbol{x})]$. Its covariance function $C_Y(\mathbf{x}_1,\mathbf{x}_2)=\langle Y'(\mathbf{x}_1)Y'(\mathbf{x}_2)\rangle$, where the perturbation $Y'(\boldsymbol{x})$ is defined as $Y'(\mathbf{x})=Y(\mathbf{x})-\langle Y(\mathbf{x})\rangle$ and $\langle\,\rangle$ represents the mean operator, is positive definite. The basic idea of the KL decomposition is to decompose the covariance function $C_Y(\boldsymbol{x}_1,\boldsymbol{x}_2)$ as,

$$C_Y(\boldsymbol{x}_1,\boldsymbol{x}_2)=\sum_{n=1}^{\infty}\lambda_n f_n(\boldsymbol{x}_1)f_n(\boldsymbol{x}_2), \qquad (3)$$

where λ_n and $f_n(\boldsymbol{x})$ are eigenvalues and deterministic eigenfunctions, respectively. The mean-removed term $Y'(\boldsymbol{x})$ can be expanded in terms of λ_n and $f_n(\boldsymbol{x})$,

$$Y'(\boldsymbol{x})=\sum_{n=1}^{\infty}\xi_n\sqrt{\lambda_n}f_n(\boldsymbol{x}), \qquad (4)$$

where ξ_n are the orthogonal standard Gaussian random variables. Since eigenvalues λ_n and their eigenfunctions $f_n(\boldsymbol{x})$ always appear together, in the following derivations, we define new functions $\tilde{f}_n(\boldsymbol{x})=\sqrt{\lambda_n}f_n(\boldsymbol{x})$ and then the tilde over f_n is dropped for simplicity.

Karhunen-Loéve Decomposition-Based Moment Equations (KLME)

In the KLME approach, head is first decomposed with a perturbation expansion as,

$$h(\boldsymbol{x},t)=\sum_{m=0}^{\infty}h^{(m)}(\boldsymbol{x},t), \qquad (5)$$

where $h^{(m)}(\boldsymbol{x},t)$ is m^{th}-order head in terms of σ_Y, the standard deviation of log hydraulic conductivity. Substituting (5) and Taylor expansion of $\exp[Y'(\boldsymbol{x})]$ into (1) – (2), collecting terms at different expansion orders, and then dropping the spatial and temporal indices for simplicity, one obtains,

$$\nabla_{xy}\cdot[K_G h_B^{(0)}\nabla_{xy}h^{(0)}]+g_u+K_G\frac{\partial h^{(0)}}{\partial z}=S_y\frac{\partial h^{(0)}}{\partial t}, \tag{6}$$

$$\nabla\cdot[K_G\nabla h^{(0)}]+g_c=S_s\frac{\partial h^{(0)}}{\partial t}, \tag{7}$$

and in general at m^{th}-order, $m \geq 1$,

$$\nabla_{xy}\cdot[K_G h_B^{(0)}\nabla_{xy}h^{(m)}]+K_G\frac{\partial h^{(m)}}{\partial z}+g_u^{(m)}=S_y\frac{\partial h^{(m)}}{\partial t}, \tag{8}$$

$$\nabla\cdot[K_G\nabla h^{(m)}]+g_c^{(m)}=S_S\frac{\partial h^{(m)}}{\partial t}, \tag{9}$$

where

$$g_u^{(m)}=\nabla_{xy}\cdot[K_G\sum_{k=1}^{m}\sum_{i=0}^{k}\frac{Y'^{k-i}}{(k-i)!}h_B^{(i)}\nabla_{xy}h^{(m-k)}]+K_G\sum_{k=1}^{m}\frac{Y'^k}{k!}\frac{\partial h^{(m-k)}}{\partial z}, \tag{10}$$

$$g_c^{(m)}=\nabla\cdot[\sum_{k=1}^{m}K_G\frac{Y'^k}{k!}\nabla h^{(m-k)}], \tag{11}$$

and $K_G(\boldsymbol{x})=\exp[<Y(\boldsymbol{x})>]$ is the geometric mean of $Y(\boldsymbol{x})$. Instead of working on the above equations directly in previous ME approaches (Zhang and Lu, 2002), in the KLME scheme we further expand $h^{(m)}(\boldsymbol{x},t)$ as,

$$h^{(m)}=\sum_{i_1,i_2,\ldots,i_m=1}^{\infty}(\prod_{j=1}^{m}\xi_{i_j})h_{i_1i_2\cdots i_m}^{(m)}, \tag{12}$$

where $h_{i_1i_2\cdots i_m}^{(m)}$ are deterministic functions to be determined; i_1, i_2, …, i_m are referred to as modes at the m^{th} order. Substituting (12) and (4) into (8) – (11) and dropping the independent set $\{\xi_{i_1}\xi_{i_2}\ldots\xi_{i_m}\}$, one obtains,

$$\nabla_{xy}\cdot[K_G h_B^{(0)}\nabla_{xy}h_{i_1i_2\cdots i_m}^{(m)}]+K_G\frac{\partial h_{i_1i_2\cdots i_m}^{(m)}}{\partial z}+g_{u_{i_1i_2\ldots i_m}}^{(m)}=S_y\frac{\partial h_{i_1i_2\ldots i_m}^{(m)}}{\partial t}, \tag{13}$$

$$\nabla\cdot[K_G\nabla h_{i_1i_2\cdots i_m}^{(m)}]+g_{c_{i_1i_2\ldots i_m}}^{(m)}=S_s\frac{\partial h_{i_1i_2\cdots i_m}^{(m)}}{\partial t} \tag{14}$$

where

$$\begin{aligned} g_{u_{i_1i_2\cdots i_m}}^{(m)}=&\nabla_{xy}\cdot K_G\sum_{k=1}^{m}\sum_{i=0}^{k}\left[\frac{(m-k+i)!}{m!}\sum_{P_{i_1,i_2,\ldots,i_m}}\prod_{j=1}^{k-i}f_{i_j}h_{i_{k-i+1}i_{k-i+2}\ldots i_k}^{(i)}\nabla_{xy}h_{i_{k+1}\ldots i_m}^{(m-k)}\right]\\ &+K_G\sum_{k=1}^{m}\frac{(m-k)!}{m!}\sum_{P_{i_1,i_2,\ldots,i_m}}\prod_{j=1}^{k}f_{i_j}\frac{\partial h_{i_{k+1}\ldots i_m}^{(m-k)}}{\partial z}\end{aligned} \tag{15}$$

$$g_{c_{i_1i_2\ldots i_m}}^{(m)}=\nabla\cdot K_G\sum_{k=1}^{m}\left[\frac{(m-k)!}{m!}\sum_{P_{i_1,i_2,\ldots,i_m}}\prod_{j=1}^{k}f_{i_j}\nabla h_{i_{k+1}\ldots i_m}^{(m-k)}\right]. \tag{16}$$

Equations (6), (7), (13), and (14) have been formulated in the same structure as the original flow equations such that MF2K can be directly applied as the solver. Solving these equations is a sequential process as higher-order *g* terms (implemented using the well package in MF2K) depend on lower-order solutions (Figure 1). The appropriate solution procedure is: 1) at the current time step, solving the zeroth-order equations, 2) solving (13) and (14) for $h_{i_1i_2\cdots i_m}^{(m)}$ at m = 1, 2, 3, …, recursively for different modes i_1, i_2, …, i_m, 3) computing the means and variances of heads and fluxes, and 4) adding a time increment and repeat steps 1) – 3), if needed. The mean heads and head variances are calculated as [Zhang and Lu, 2004],

$$< h > \approx h^{(0)} + \sum_{i=1}^{\infty} h_{ii}^{(2)}, \quad \sigma_h^2 \approx \sum_{i=1}^{\infty} [h_i^{(1)}]^2 + 2\sum_{i,j=1}^{\infty} [h_{ij}^{(2)}]^2 + 6\sum_{i,j=1}^{\infty} [h_i^{(1)} h_{ijj}^{(3)}]. \quad (17)$$

where the first term on the right-hand side of $< h >$ is the zeroth-order mean head solution and the second term represents the second-order corrections; for σ_h^2 the first term is the head variance up to the first order in σ_Y^2, and the second and third terms represent the second-order corrections. Flux statistics can be computed in a similar manner (Lu and Zhang, 2004).

Compared to the conventional ME approach, the KLME method has two distinctive advantages. First, unlike the conventional ME approach, the KLME method does not require solving directly the covariance equations such as head covariances and head-permeability cross covariances, whose computations are proportional to the number of model dimensions (N), thereby significantly reducing the computational efforts especially for large-scale problems. Second, as demonstrated in the above derivations, higher-order terms can be easily incorporated into the KLME method. The conventional ME approach usually approximates the covariance of flow quantities only up to the first order in σ_Y^2 because the computational burden increases drastically when higher-order corrections are implemented. For instance, to obtain the hydraulic head variance up to second-order in σ_Y^2, one needs to solve equations for terms such as $< Y'(\boldsymbol{x_1})Y'(\boldsymbol{x_2})h'(\boldsymbol{x_3},t) >$, which generally requires solving the partial differential equations for N^2 times.

ILLUSTRATIVE EXAMPLE

The MODFLOW-STO model developed in this study is validated and its efficiency and accuracy have been demonstrated with comparisons to traditional MCS in a series of hypothetical numerical experiments. In this section we present a 3-D unconfined flow example in which a total of 5000 realizations are used in the MCS; in the KLME method, the number of modes at the first three orders is 100, 20 and 10, respectively, resulting in a total of 1 (zeroth-order) + 100 (first-order) + 210 (second-order) + 220 (third-order) = 531 model simulations.

Problem Description

The schematic diagram of model setup is shown on Figure 2. A cuboid of 30 m × 10 m × 9 m is uniformly discretized into a block-centered finite-difference mesh of 121 columns by 40 rows by 3 layers. The size of each cell is 0.25 m × 0.25 m × 3 m. The western and eastern boundaries have constant heads of 8.5 m and 7.5 m, respectively. There is no flow across all other borders. A local recharge is applied at rate 0.3 m/d in a region of 10 rows by 30 columns (x: 11.125 ~ 18.625 m; y: 3.75 ~ 6.25 m). Here the recharge rate is assigned a high value such that its effects can be demonstrated better. A well is located at the center of domain (column 61, row 21, and layer 2) and pumped at a rate of 3 m^3/d. Transient simulation is conducted with S_y = 0.1 for the water-table layer and S_s =1.0E-4 for confined layers. The log conductivity field has a zero mean (K_G =1.0 m/d) and follows a separable exponential covariance function with variance σ_Y^2 = 1.0 and correlation lengths $\eta_x = \eta_y = \eta_z$ = 5.0 m.

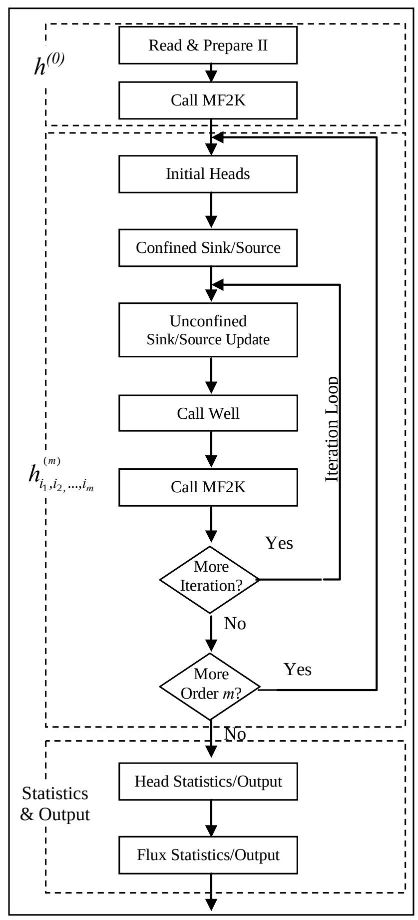

Figure 1. Computational scheme for MODFLOW-STO

Results and Discussions

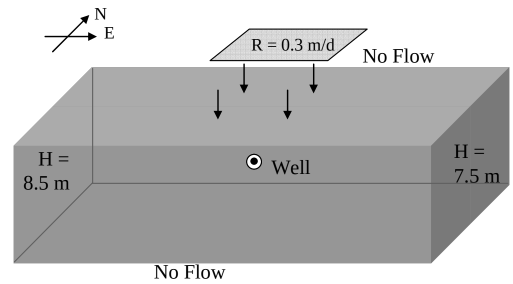

Figure 2. Schematic Problem Setup

Figure 3 shows the means and variances of heads and fluxes calculated at the end of simulation from the KLME approach in MODFLOW-STO and the MCS. Results are shown along the 20th row of top unconfined layer. Recharge and the pumping well have a big impact on flow statistics. For the mean heads and fluxes, the KLME and MCS results are in close agreement. For head variances, the first-order values calculated by KLME undershoot the MCS results in the vicinity of recharge, and adding second-order corrections improves solution accuracy significantly. For flux variances, there is a noticeable underestimation by the both orders of results in the KLME approach; nonetheless, the overall trend between KLME and MCS is consistent. It can be seen from this example that the KLME approach implemented in MODFLOW-STO can offer one order of magnitude reduction in the computation effort and yet is accurate in providing the stochastic flow solutions under general field conditions.

CONCLUSIONS

This paper has presented a stochastic version of MODFLOW, referred to as MODFLOW-STO, for simulating stochastic flow problems based on a Karhunen-Loéve decomposition based moment-equation (KLME) approach. The accuracy and efficiency of this model have been validated with comparisons to the classical Monte Carlo simulations (MCS) in a 3-D unconfined flow example.

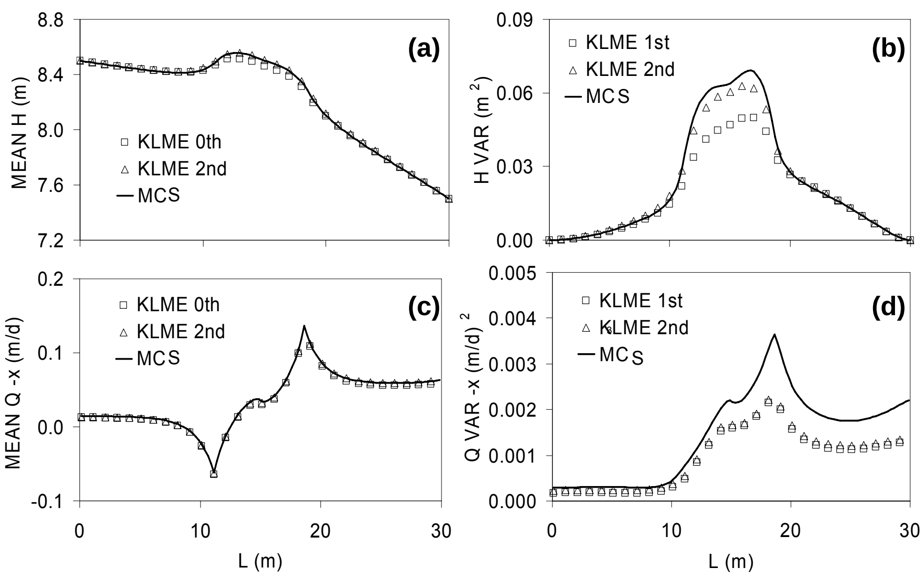

Figure 3. The means and variances of heads and fluxes calculated from KLME and MCS

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